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STEM

## Microstructure Development During Compaction of Granular Systems

Student researcher: Chen Shang, Junior

Granular materials are the second most manipulated materials in industry today. They are easy to transport and more suitable than most other materials for the processing of a wide range of modern and traditional materials. Having a better understanding of the microstructure development and evolution during the compaction of granular systems will enable better design and control of the manufacturing process. Modeling this process requires a particle mechanics approach to describe each individual particle in the powder bed and to determine inter-particle contact forces and deformations. A first step in the direction of formulating a predictive model is restricting attention to elastic deformations—that is, using the Hertz contact law for small deformations and a nonlocal contact elastic formulation for moderate deformations and high levels of particle confinement. Nonlocal contact formulations remain predictive at high levels of confinement, or low porosity, by removing the classical assumption that contacts between particles are formulated locally as independent pair interactions.

Powder Compaction, a nanoHUB tool (http://dx.doi.org/10.4231/D33N20F7K), was developed with the educational and scientific purpose of modeling the compaction of binary mixtures of monodispersed elastic particles. The user can select the number of particles, elastic material properties, and volume fraction of the mixture, together with the contact model to be employed: Hertz law or nonlocal contact formulation (top left of the figure). The main outputs are (i) the compaction plot—that is, punch pressure and die-wall reaction versus relative density (figure top right); (ii) 3-D images showing the particle structure evolution during compaction (figure bottom); (iii) the evolution of the mean coordination number—that is, the average number of particles that are in contact with a single particle; and (iv) the probability distribution of contact forces. The tool highlights that results for the nonlocal contact formulation largely depart from those for Hertzian contact at relative densities larger than 0.70 and for nearly incompressible materials (i.e., for Poisson ratio close to one-half). The tool can also be used to generate mixture plots (i.e., compaction pressure versus composition) for a given relative density or porosity. These mixtures behave nonlinearly, and thus the elucidation of mixture rules for general powders remains an area of research.

*Research advisor Marcial Gonzalez writes, "Prediction of microstructure formation and evolution during powder compaction processes is essential to enable the systematic optimization of many products currently manufactured in the industry and the development of new ones. Chen developed an online tool that provides scientists and educators with worldwide access to computational models that predict some of these microstructural features."*

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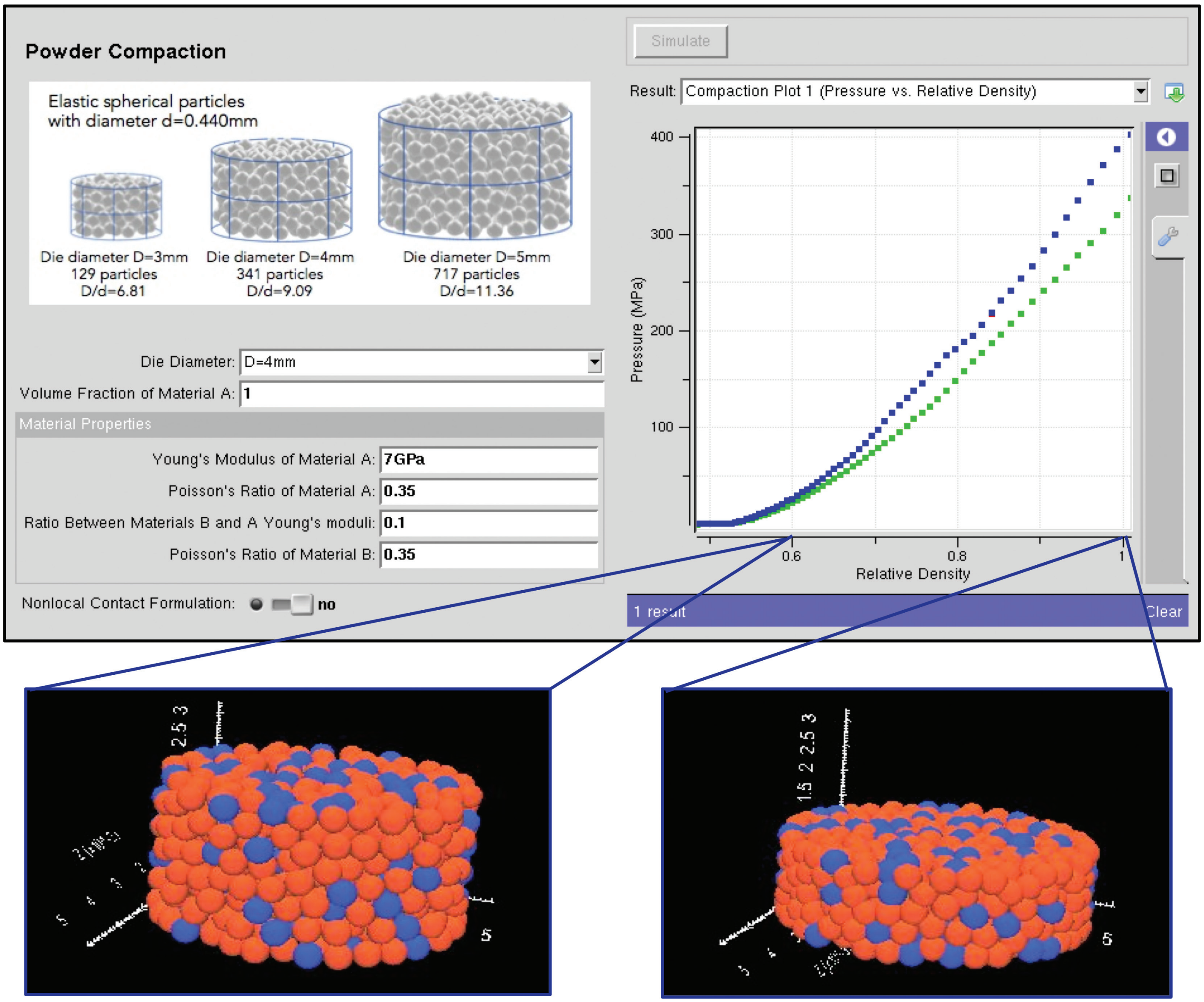


GUI of the powder compaction tool with key outputs: compaction plot (top right) and 3-D structure of the mixture at a relative density of 0.6 (bottom left) and at a relative density of 1 (bottom right).

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